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Optimization of DI diesel engine parameters fueled with *iso*-butanol/diesel blends – Response surface methodology approach

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HIGHLIGHTS

- Minimizing smoke and NOx emissions simultaneously with maximum BTE and minimum BSFC.
- Optimum combination of factors with highest desirability is (0.969).
- Validation of the models developed using RSM.
- Effect of the injection pressure, injection timing and EGR on performance and emissions for all blends.

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ABSTRACT

Iso-butanol is a naturally occurring 4-carbon alcohol that can be obtained by processing organic crops like corn and sugarcane. An experimental and statistical investigation is carried out to analyze the effects of injection-pressure, timing and exhaust gas recirculation (EGR) on performance and emissions of a DI diesel engine fuelled with 40% by vol. of *iso*-butanol/diesel blend. Response surface methodology was used to model all measured responses like nitrogen oxides (NOx), smoke opacity, brake thermal efficiency (BTE) and brake specific fuel consumption (BSFC). Analysis of variance (ANOVA) revealed that all developed models were statistically significant. Interactive effects between injection pressure, injection timing and EGR for all blends were analyzed using response surface plots that were plotted using developed regression models. Optimization was performed using desirability approach of the RSM with an objective to minimize NOx and smoke emissions simultaneously with maximum BTE and minimum BSFC. *Iso*-butanol/diesel blend injected at 240bar pressure, 23°CA bTDC under 30% EGR was predicted to be optimum for this particular engine. The predicted combination was validated by confirmatory tests and the error in prediction was found to be within 4%.

1. Introduction

Diesel engines are popular energy conversion devices because of their higher thermal efficiency, higher torque capability and higher durability when compared to gasoline engines [1]. High NOx and PM emissions remain as main obstacles in the research and development of next generation diesel engines [2]. NOx causes smog [3], ground-level ozone [4] and acid rain [5]. Smoke is carcinogenic [6,7] and its continuous exposure can cause various diseases to human [8–12]. To address these issues, diesel engine researchers attempt to reduce emissions often by modifying engine design parameters and using after-treatment devices.

EGR and retarded injection timing were often used to suppress NOx formation [13]. Using EGR reduces peak combustion temperatures in the combustion chamber which encourages NOx formation and controls the combustion phasing [14]. Retarding the injection timing also lengthens the ignition delay and could result in further reduction of NOx emissions with a slight penalty in smoke and fuel consumption [15,16]. Diesel reformulation with biofuels is a popular option among researchers because it is a practical approach that requires few modifications to the existing engine layout. Adding biofuels to fossil diesel increases the renewable fraction in the cylinder and improves energy security. Further

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the presence of fuel-bound oxygen in biofuels increases the availability of oxygen even in fuel-rich zones during combustion. Recently, investigations on long-chain alcohols like *iso*-butanol and pentanol are in spotlight because of their higher energy content, higher cetane number, better solubility with diesel and less water-absorbing nature than their short-chain counterparts like ethanol and methanol. Table 1 presents the fuel properties of *iso*-butanol in comparison with other lower alcohols. *Iso*-butanol is a 4-carbon alcohol which can be obtained by fermentation of organic crop material like corn and sugarcane which has already captured energy from the sun and stored it in the form of chemical energy [2]. *Iso*-butanol is a naturally occurring alcohol like its popularly researched counterpart '*n*-butanol', but presents several advantages over it. In the recent years, *iso*-butanol is increasingly favored by the industry because *n*-butanol production technology is handicapped by high energy cost due to its production in low concentrations and significant volumes of water processed even with new Clostridia strains [17]. *Escherichia coli* can be engineered to produce 22 g/L of *iso*-butanol, a value that exceeded most of the native n-butanol production quantities using the valine biosynthetic pathway [18,19]. Moreover, optimization of *iso*-butanol production from glucose has achieved a yield of 50 g/L using the valine pathway [20] when compared to the modified CoA (Coenzyme A) pathway that yielded only 30 g/L of *n*-butanol [21] in lab-scale fermenters with engineered *Escherichia coli*. Another advantage is that existing ethanol plants that use corn, sugarcane and cellulose as feedstock can be re-purposed to produce *iso*-butanol by just modifying the bio-catalyst as demonstrated by Gevo [22].

Unlike *n*-butanol, which is heavily researched in the last 5 years, very few studies have investigated the use of *iso*-butanol in diesel engines till date. Al-Hasan et al. [23] investigated the performance of four *iso*-butanol/diesel blends (10, 20, 30 and 40%) in a single-cylinder diesel engine and reported a drop in performance with increase in *iso*-butanol content in the blends. Karabektas et al. [24] reached identical conclusions with respect to engine performance using four *iso*-butanol/diesel blends (5, 10, 15 and 20%) in a single-cylinder diesel engine. They reported reduction in NOx and CO emissions with increase in *iso*-butanol fraction in the blends. Ozsezan et al. [25] used three *iso*-butanol/diesel blends (5, 10 and 15% by vol) in a six-cylinder diesel engine and have shown that smoke and NOx emissions decreased with increasing *iso*-butanol fraction in the blends. Gu et al. [26] concluded that the combination of a low EGR and retarded injection timing can reduce smoke and NOx emissions simultaneously while maintaining an acceptable fuel economy. They found that *iso*-butanol exhibited higher peaks of in-cylinder pressure and heat release rate when compared to n-butanol. Zheng et al. [27] studied the effects of four butanol isomers blends (n-butanol, *iso*-butanol, *sec*-butanol and ter-butanol) in diesel (20 and 40%) on performance and emissions in a direct-injection diesel engine with high EGR rates. They found that *iso*-butanol/diesel blends presented longest ignition delay and produced lowest smoke emissions when compared to other isomers. Rajesh et al. [2,28] reported that the combination of EGR rates up to 30%, *iso*-butanol addition of up to 40% and retarded injection timing by 2°CA bTDC can simultaneously reduce NOx and smoke emissions.

In this context, the present study utilizes three factors namely, injection pressure, injection timing and EGR for optimizing emission and performance characteristics of a single cylinder DI diesel engine. Three levels of each factor were chosen. Three injection pressures (200, 220 and 240bar), Three EGR rates (10, 20 and 30%) and three injection timings (19°, 21° and 23°CA bTDC) were used to control combustion phasing. A 3 × 3 full factorial design was used to design the experiments. Response surface methodology (RSM) was employed to acquire optimum combination of the above factors to minimize NOx and smoke emissions with maximum possible BTE and minimum BSFC. Previous studies have analyzed the effect of injection timing and EGR with *iso*-butanol/diesel blends up to 30% by vol. in diesel. However an optimal combination of these emission and performance parameters and the individual effects of factors like injection timing, injection pressure and EGR have not been analyzed using robust optimization techniques. The knowledge of the effects of the above factors on emissions and performance could enable engine manufacturers to make informed decisions on choosing appropriate combination.

The objectives of this study are: (i) to quantify the main and interactive effects of injection pressure, EGR and injection timing on engine performance and emission characteristics, (ii) to develop regression models for NOx, smoke opacity, BTE and BSFC using the full factorial design that can accurately describe the experimental data, and (iii) to obtain an optimum combination of the considered factors to minimize NOx and smoke with maximum possible efficiency using desirability approach.

2. Materials and methods

2.1. Test fuels

Ultra low sulfur diesel (ULSD) is the reference fuel for this study and was purchased from an outlet of Shell Petroleum at Chennai. *iso*-butanol, an isomer of butanol (C_4H_9OH), having a branched chain structure with a hydroxyl group at the terminal carbon (as shown in Fig. 1) is utilized in this study. Analytical grade *iso*-butanol (CAS No: 78-83-1) certified to a purity of 98.5%, was procured from a local supplier. The impurities present were identified to be *iso*-butyraldehye (0.03%), acetone (0.02%), water (0.1%) and butyric acid (0.005%). *Iso*-butanol was blended with ULSD by a volume ratio of 40/60 and is referred to as ISB40. This blend was kept undisturbed and was found stable with no phase separation over a

Table 1
Fuel properties.[a]

Properties	Diesel	Methanol	Ethanol	*Iso*-butanol
Molecular weight (kg/kmol)	190–211.7	32.04	46.07	74.12
O (% wt)	0	49.93	34.73	21.59
Solubility (g/L)	Immiscible	Miscible	Miscible	77
Cetane number	52	5	8	<15
Self-ignition temperature (°C)	254–300	463	420	415
Density (kg/m^3) at 15 °C	835	791.3	789.4	802
Viscosity at 40 °C (mm/s^2)	2.72	0.58	1.13	2.63
Lower heating value (MJ/kg)	42.49	19.58	26.83	33.64
Latent heat of evaporation (kJ/kg)[a]	270–375	1162.64	918.42	684
Vapor pressure (mmHg)	0.4	127	55	10.4
Boiling point (°C)	180–360	64.7	78.3	108
Flash point (°C)	>55	11–12	17	28

[a] Data have been taken from Ref. [2,23–26].